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Atmospheric Chemistry and Physics Discussions

Interactive comment on "CFD Modeling of Reactive Pollutants Dispersion in Simplified Urban Configurations with Different Chemical Mechanisms" *by* Beatriz Sanchez et al.

Anonymous Referee #1

Received and published: 14 July 2016

In the paper, Sanchez et al. study how NOx-Ozone-VOC chemistry over a city can be best simulated, accounting for reliability and computer time. The paper describes three general approaches: a setup where NOx and Ozone are passive tracers (considering that transport and mixing in street canyons are relatively compared with chemistry), a setup with simple chemistry (the photostationary state, NO2 + O2 + hv <-> NO + O3, computationally efficient, most relevant chemical processes), and a setup with an expanded set of chemical equations derived from the RACM scheme. The authors test the setup in an idealized 2D and 3D representation of a (number of) street canyons, with high and low zenith angle and corresponding solar radiation intensity (winter and summer situations, or low and high background Ozone concentrations), and VOC/NOx

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emissions rates of 1/5 and 1/2. Furthermore, they test the influence of wind speed (u = 0.45 m.s-1 and u=0.23 m.s-1). The authors thus choose to manipulate a large number of input variables, which results in a large number of different results. This is both a strong and weak point of the paper. It is strong because the results are put in a broad perspective. It is weak because it is difficult to keep track of all the different results. I suggest that the authors make an effort to create a better overview of the different experiments, and possibly introduce acronyms for them, and use them as titles in the figures and tables. Nevertheless, the authors come to clear and understandable conclusions:

- Wind speed determines the vertical exchange rate, and therefore the influx of background Ozone.

- The choice of chemical scheme is more important in the situations with high O3 concentrations

- In high wind and high background O3 concentrations, it is essential to use an expanded set of chemical equations. The impact obviously increases with the VOC emission rate.

In my opinion, the paper describes a very well-organised set of experiments, which yield clear conclusions. Although the experiments already encompass a large number of manipulations, the conclusions remain somewhat qualitative (in conditions of high/low Ozone, wind speed, VOC emission rates). As a result, the results will be difficult to apply directly by other researchers.

It would be convenient if the authors could work towards specifying threshold values for those variables or describing the sensitivity of the results to these variables. I understand that this would involve doing the same experiments with a broader range of the variables and/or more and smaller step sizes. Probably this also includes using non-idealized street geometry. I am not suggesting that the authors do all that for the current paper. But they should include clear recommendations on how to turn the

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qualitative conclusions into quantitative and applicable results.

I recommend publication of this paper in Atmospheric Chemistry and Physics with minor revisions: 1) create a better overview over the many different experiments and 2) include recommendations on how to come to quantitative and applicable results. The paper also needs English grammar editing.

Detailed comments

- 'researches': research is never a plural in English. Better use 'studies'.

Abstract

- line 12: explain the role of wind speed

- line 14: founded > found

- line 14: related with > related to

- line 16-17: rephrase

Page 2

- line 19: '. . . we found IT more . . .'

- line 29: '.. in urban areas IT becomes more . . .'

- line 33: 'marked'? Not clear what you mean

- line 35: 'O3 sensitivity', do you mean the sensitivity of O3 to ??? or the sensitivity of the results to O3? This is not clear.

Page 3:

- line 3: '. . . whereby increasing the wind speed enhances the exchange with the overlying air. . .'

- line 3: strengthens

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- line 23: ‘The aim of this work is to determine in which conditions it is essential . . .’

Page 4, line 8: JNO2 and k are not shown in the equations

Page 5:

- Line 11: ‘As well. . .’ > ‘Also. . .’

- Line 25-end: rephrase

Page 6:

- Section 3.2: restructure this section. It is now not very well organised. It sounds like new experiments are introduced continuously with another set of manipulated variables. I think it would be good to introduce a table with an overview over all the different experiments right in the beginning, and then use this section to explain the individual experiments and their mutual relationships. I found it somewhat confusing that you refer to the low/high background O3 concentration experiments as winter/summer and high/low zenith angle experiments (I assume these are the same experiments). You might also consider introducing descriptive acronyms for the experiments, which you could use in the titles of the figures and tables and in the text.

- Line 17: are the symmetric conditions also applied to the concentrations?

- Line 21: ‘within the typical range of values. . .’

- Line 23: ‘two background O3 concentrations’: specify which, this has not yet been introduced at this stage. Page 7:

- Line 4-5: the NO/NO2 concentrations also depend on the intensity of turbulent mixing in the boundary layer, e.g. the difference between clear and cloudy days, or strong/weak inversion. How has this been addressed?

- Line 21: ‘from a well-established chemical box model’: describe which one in some words. After reviewing the paper I do not have a clear idea on where the results of this

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box model are used. Is this an essential part of the paper?

Page 9:

- Line 13: I found the use of the word ‘canopy’ confusing. E.g. in page 10, line 11 you write ‘below the canopy’. This suggests that you simulate concentrations below trees. Is this true? Please clarify. How tall is the canopy?

- Line 14: ‘. . ., and the pollutants reside longer in the street. . .’

- Line 18: ‘To facilitate the comparison. . .’

- Line 19: is the source emission rate Q expressed per unit area? Otherwise the normalisation with A_em is not needed.

- Line 20: It would make sense to use C_N instead of Cnorm, because later on you use [NO2]N etc.

- Line 20: describe L

Page 10:

- Line 4: ‘the effect of . . . emission ratio settings ON the amount. . .’

- Line 5: ‘. . . fixed emission rates. . .’

- Line 11-13: ‘On the other hand. . .’ suggest that the new sentence is in contradiction with the previous one, but this is not the case.

- Could you explain why in the low O3 case the VOC emissions do not make much difference?

Page 11, line 11 to end: this is discussion, not results. I would expect that you describe the difference between the 2D and 3D experiments here.

Page 12:

- Line 4: on accurate way > accurately.

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- Line 9: ‘without hardly differences’ is a double negative: ‘with hardly any differences’ or ‘without any differences’ or ‘without large differences’

Page 13:

- Line 14: slightly minor/major: I think you mean slightly smaller or larger?

- Line 25: IN this way

- Line 33: reacts > react

Page 14: Line 2-4: rephrase

Page 15:

- Line 4-5: rephrase

- Line 6: rise > increase

- Line 8-20: Can you make this part more quantitative, and include recommendations to direct further research?

- The subject of computation time is not addressed here. Perhaps implicitly, but not explicitly.

Table 2: specify the background concentrations (instead of high/low)

Figures: The fonts in the figure titles/axes/legends are extremely small.

Figure 6: subplot e should be the same as 4e? They refer to the same experiment if I understand it correctly.

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